On modified Newton iterations for SPARK methods applied to constrained systems in mechanics

Laurent O. Jay

Department of Mathematics, 14 MacLean Hall, The University of Iowa, Iowa City, IA 52242-1419, USA.
E-mail: `ljay@math.uiowa.edu` *and* `na.ljay@na-net.ornl.gov`.

Abstract. The application of modified Newton iterations to the solution of SPARK methods applied to a large class of overdetermined differential-algebraic equations (ODAEs) is described in some details. These ODAEs include the formulation of systems in mechanics with holonomic and nonholonomic constraints.

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1. INTRODUCTION

We consider the following class of systems of implicit, partitioned, additive, and overdetermined differential-algebraic equations (ODAEs)

$$\frac{d}{dt}y = v(t,y,z), \quad \frac{d}{dt}p(t,y,z) = f(t,y,z,\psi) + r(t,y,\lambda), \quad 0 = g(t,y), \quad 0 = g_t(t,y) + g_y(y)v(t,y,z), \quad 0 = k(t,y,z) \quad (1)$$

where we assume that

$$\begin{pmatrix} p_z & -r_\lambda & -f_\psi \\ g_y v_z & O & O \\ k_z & O & O \end{pmatrix} \quad \text{is nonsingular,} \qquad (2)$$

and that

$$\begin{pmatrix} p_z & -r_\lambda \\ g_y v_z & O \end{pmatrix} \quad \text{is nonsingular.} \qquad (3)$$

The variable $t \in \mathbb{R}$ is the independent variable, $y \in \mathbb{R}^{n_y}$ and $z \in \mathbb{R}^{n_z}$ are the *differential* variables, $\lambda \in \mathbb{R}^{n_\lambda}$ and $\psi \in \mathbb{R}^{n_\psi}$ are the *algebraic* variables. The initial values (y_0, z_0) at t_0 are assumed to be given and consistent, i.e., the constraints in (1) must be satisfied. Sufficient differentiability of the functions v, p, f, r, g, k are also assumed to ensure existence and uniqueness of a solution. The ODAEs (1) include the formulation of mechanical systems with mixed constraints of holonomic, nonholonomic, scleronomic, and rheonomic types. In mechanics the quantities y, v, p represent respectively certain coordinates, their velocities, and their momenta; the right-hand side of the second equations in (1) contains forces acting on the system; the corresponding ODAEs can be derived from the Lagrange-d'Alembert principle; λ and ψ are Lagrange multipliers associated respectively to the holonomic constraints $0 = g(t,y)$, $0 = g_t(t,y) + g_y(y)v(t,y,z)$ and to the nonholonomic constraints $0 = k(t,y,z)$.

2. (s,s)-SPARK METHODS

One step of an (s,s)-*SPARK method* applied to the system of ODAEs (1) with consistent initial values (y_0, z_0) at t_0 and stepsize h is given as follows

$$Y_i \quad = \quad y_0 + h\sum_{j=1}^{s} a_{ij} v(T_j, Y_j, Z_j) \qquad \text{for } i = 1, \ldots, s,$$

$$
\begin{aligned}
p(T_i,Y_i,Z_i) &= p(t_0,y_0,z_0) + h\sum_{j=1}^{s}\widehat{a}_{ij} f(T_j,Y_j,Z_j,\Psi_j) + h\sum_{j=0}^{s}\widetilde{a}_{ij} r(\widetilde{T}_j,\widetilde{Y}_j,\widetilde{\Lambda}_j) \quad \text{for } i=1,\ldots,s,\\
\widetilde{Y}_i &= y_0 + h\sum_{j=1}^{s}\overline{a}_{ij} v(T_j,Y_j,Z_j) \quad \text{for } i=0,1,\ldots,s,\\
0 &= g(\widetilde{T}_i,\widetilde{Y}_i) \quad \text{for } i=0,1,\ldots,s,\\
0 &= \sum_{j=1}^{s} b_j c_j^{i-1} k(T_j,Y_j,Z_j) \quad \text{for } i=1,\ldots,s-1,\\
y_1 &= y_0 + h\sum_{j=1}^{s} b_j v(T_j,Y_j,Z_j),\\
p(t_1,y_1,z_1) &= p(t_0,y_0,z_0) + h\sum_{j=1}^{s}\widehat{b}_j f(T_j,Y_j,Z_j,\Psi_j) + h\sum_{j=0}^{s}\widetilde{b}_j r(\widetilde{T}_j,\widetilde{Y}_j,\widetilde{\Lambda}_j),\\
0 &= g(t_1,y_1),\\
0 &= g_t(t_1,y_1) + g_y(t_1,y_1)v(t_1,y_1,z_1),\\
0 &= k(t_1,y_1,z_1)
\end{aligned}
$$

where

$$
t_1 := t_0 + h, \qquad T_i := t_0 + c_i h \quad \text{for } i=1,\ldots,s, \qquad \widetilde{T}_i := t_0 + \widetilde{c}_i h \quad \text{for } i=0,1,\ldots,s.
$$

For Lobatto coefficients a similar definition was proposed in [1, 2]. The definition given here is more general as it can also include for example Gauss and Radau coefficients. We have four sets of coefficients (b_j,a_{ij},c_i), $(\widehat{b}_j,\widehat{a}_{ij})$, $(\widetilde{b}_j,\widetilde{a}_{ij})$, $(\overline{a}_{ij},\widetilde{c}_i)$, where we have defined

$$
c_i := \sum_{j=1}^{s} a_{ij} \quad \text{for } i=1,\ldots,s, \qquad \widetilde{c}_i := \sum_{j=1}^{s}\overline{a}_{ij} \quad \text{for } i=0,1,\ldots,s.
$$

We assume that $\overline{a}_{0j}=0$ for $j=1,\ldots,s$ which implies that $\widetilde{Y}_0=y_0$, $\widetilde{c}_0=0$, $\widetilde{T}_0=t_0$, and $0=g(\widetilde{T}_0,\widetilde{Y}_0)=g(t_0,y_0)$ is thus automatically satisfied. We also assume that $\overline{a}_{sj}=b_j$ for $j=1,\ldots,s$ which implies that $\widetilde{Y}_s=y_1$, $\widetilde{c}_s=1$, and $\widetilde{T}_s=t_1$. Hence, from $0=g(\widetilde{T}_s,\widetilde{Y}_s)$ the condition $0=g(t_1,y_1)$ is also automatically satisfied. Notice that the coefficients $(b_j,c_j)_{j=1}^{s}$ and $(\widetilde{b}_j,\widetilde{c}_j)_{j=0}^{s}$ generally correspond to two distinct quadrature formulas. We assume $b_i \neq 0$, $c_i \neq c_j$ for $i \neq j$, and the matrix A to be invertible. We use the following notation, $\mathbb{1}_s := (1,1,\ldots,1)^T \in \mathbb{R}^s$, $0_s := (0,0,\ldots,0)^T \in \mathbb{R}^s$, $e_{s+1} := (0,0,\ldots,0,1)^T \in \mathbb{R}^{s+1}$, $I_s := \operatorname{diag}(1,1,\ldots,1) \in \mathbb{R}^{s\times s}$, $C := \operatorname{diag}(c_1,c_2,\ldots,c_s) \in \mathbb{R}^{s\times s}$, and we define

$$
\alpha := \begin{pmatrix} A \\ b^T \end{pmatrix} \in \mathbb{R}^{(s+1)\times s}, \quad \widehat{\alpha} := \begin{pmatrix} \widehat{A} \\ \widehat{b}^T \end{pmatrix} \in \mathbb{R}^{(s+1)\times s}, \quad \widetilde{\alpha} := \begin{pmatrix} \widetilde{A} \\ \widetilde{b}^T \end{pmatrix} \in \mathbb{R}^{(s+1)\times(s+1)}.
$$

We assume that $\widetilde{\alpha}$ is invertible. We also define

$$
\widetilde{Q} := \begin{pmatrix} I & 0_s \end{pmatrix} + AM^{-1}\mathbb{1}_s \begin{pmatrix} -b^T A^{-1} & 1 \end{pmatrix} \in \mathbb{R}^{s\times(s+1)}
$$

where we assume that

$$
M := \begin{pmatrix} b^T \\ b^T - b^T A \\ \vdots \\ b^T - (s-1) b^T C^{s-2} A \end{pmatrix} \in \mathbb{R}^{s\times s} \quad \text{is invertible.}
$$

We define

$$
\gamma^T = \begin{pmatrix} \widetilde{\gamma}^T & \gamma_{s+1} \end{pmatrix}^T := \gamma_{s+1} \begin{pmatrix} -b^T A^{-1} & 1 \end{pmatrix} \neq 0 \in \mathbb{R}^{s+1}
$$

which satisfies the s orthogonality conditions $\gamma^T \alpha = 0$. We define the invertible matrix Q by

$$
Q := \begin{pmatrix} \widetilde{Q} \\ \gamma^T \end{pmatrix} \in \mathbb{R}^{(s+1)\times(s+1)}
$$

and the matrix $\check{Q}$ by

$$\check{Q} := Q \begin{pmatrix} \check{A}^{-1} & 0_s \\ 0_s^T & 1 \end{pmatrix} \in \mathbb{R}^{(s+1)\times(s+1)}$$

where we assume that

$$\check{A} := \begin{pmatrix} \overline{a}_{11} & \cdots & \overline{a}_{1s} \\ \vdots & \ddots & \vdots \\ \overline{a}_{s1} & \cdots & \overline{a}_{ss} \end{pmatrix} \in \mathbb{R}^{s\times s} \quad \text{is invertible}$$

and that $e_{s+1}^T Q\widehat{\alpha} = 0_s$, for example by having $\widehat{\alpha} = \alpha$. More details can be found in [3, 4, 5].

2.1. Reformulation of (s,s)-SPARK methods

To solve the nonlinear system of equations for (s,s)-SPARK methods we consider the application of modified Newton methods. In order to obtain an efficient implementation requiring only the decomposition of the 2 matrices in (2) and (3) we reformulate the nonlinear system of equations of (s,s)-SPARK methods equivalently as follows

$$0 = \begin{pmatrix} Y_1 \\ \vdots \\ Y_s \\ y_1 \end{pmatrix} - \mathbb{1}_{s+1} \otimes y_0 - h(\alpha \otimes I_{n_y}) \begin{pmatrix} v(T_1,Y_1,Z_1) \\ \vdots \\ v(T_s,Y_s,Z_s) \end{pmatrix}, \tag{4}$$

$$0 = (Q \otimes I_{n_z}) \left(\begin{pmatrix} p(T_1,Y_1,Z_1) \\ \vdots \\ p(T_s,Y_s,Z_s) \\ p(t_1,y_1,z_1) \end{pmatrix} - \mathbb{1}_{s+1} \otimes p(t_0,y_0,z_0) - h(\widehat{\alpha} \otimes I_{n_z}) \begin{pmatrix} f(T_1,Y_1,Z_1,\Psi_1) \\ \vdots \\ f(T_s,Y_s,Z_s,\Psi_s) \end{pmatrix} - h(\widetilde{\alpha} \otimes I_{n_z}) \begin{pmatrix} r(\widetilde{T}_1,\widetilde{Y}_1,\widetilde{\Lambda}_1) \\ \vdots \\ r(\widetilde{T}_s,\widetilde{Y}_s,\widetilde{\Lambda}_s) \end{pmatrix} \right), \tag{5}$$

$$0 = (\check{Q} \otimes I_{n_\lambda}) \begin{pmatrix} \frac{1}{h} g\left(\widetilde{T}_1, y_0 + h\sum_{j=1}^s \overline{a}_{1j} v(T_j,Y_j,Z_j)\right) \\ \vdots \\ \frac{1}{h} g\left(\widetilde{T}_s, y_0 + h\sum_{j=1}^s \overline{a}_{sj} v(T_j,Y_j,Z_j)\right) \\ g_t(t_1,y_1) + g_y(t_1,y_1) v(t_1,y_1,z_1) \end{pmatrix}, \tag{6}$$

$$0 = (\widetilde{Q} \otimes I_{n_\psi}) \begin{pmatrix} k(T_1,Y_1,Z_1) \\ \vdots \\ k(T_s,Y_s,Z_s) \\ k(t_1,y_1,z_1) \end{pmatrix} \tag{7}$$

where

$$\begin{pmatrix} \widetilde{Y}_0 \\ \widetilde{Y}_1 \\ \vdots \\ \widetilde{Y}_s \end{pmatrix} := \mathbb{1}_{s+1} \otimes y_0 - h(\overline{A} \otimes I_{n_y}) \begin{pmatrix} v(T_1,Y_1,Z_1) \\ \vdots \\ v(T_s,Y_s,Z_s) \end{pmatrix}.$$

2.2. Modified Jacobian and modified Newton iterations

The modified Jacobian of the nonlinear system of equations (4)-(5)-(6)-(7) can be taken as

$$\begin{pmatrix} I_{s+1}\otimes I_{n_y} & O & O & O \\ O & Q\otimes p_z & -hQ\widetilde{\alpha}\otimes r_\lambda & -hQ\widehat{\alpha}\otimes f_\psi \\ O & Q\otimes g_y v_z & O & O \\ O & \widetilde{Q}\otimes k_z & O & O \end{pmatrix}$$

where the partial derivatives $p_z, f_\psi, r_\lambda, g_y, k_z, v_z$ are evaluated for example at $t_0, y_0, z_0, \lambda_0, \psi_0$. We consider intermediate quantities to solve the linear systems of the modified Newton iterations. First we can obtain a block diagonal linear system with s matrix blocks (2) of dimension $n_z + n_\lambda + n_\psi$ for

$$\begin{pmatrix} \Delta_1^z \\ \vdots \\ \Delta_s^z \end{pmatrix} := (\widetilde{Q}\otimes I_{n_z}) \begin{pmatrix} \Delta Z_1 \\ \vdots \\ \Delta Z_s \\ \Delta z_1 \end{pmatrix}, \quad \begin{pmatrix} \Delta_1^\lambda \\ \vdots \\ \Delta_s^\lambda \end{pmatrix} := h(\widetilde{Q}\widetilde{\alpha}\otimes I_{n_\lambda}) \begin{pmatrix} \Delta\widetilde{\Lambda}_0 \\ \Delta\widetilde{\Lambda}_1 \\ \vdots \\ \Delta\widetilde{\Lambda}_s \end{pmatrix}, \quad \begin{pmatrix} \Delta_1^\psi \\ \vdots \\ \Delta_s^\psi \end{pmatrix} := h(\widetilde{Q}\widehat{\alpha}\otimes I_{n_\psi}) \begin{pmatrix} \Delta\Psi_1 \\ \vdots \\ \Delta\Psi_s \end{pmatrix}.$$

By invertibility of $\widetilde{Q}\widehat{\alpha}$ we obtain the values $\Delta\Psi_1, \ldots, \Delta\Psi_s$ from

$$\begin{pmatrix} \Delta\Psi_1 \\ \vdots \\ \Delta\Psi_s \end{pmatrix} = \frac{1}{h}((\widetilde{Q}\widehat{\alpha})^{-1}\otimes I_{n_\psi}) \begin{pmatrix} \Delta_1^\psi \\ \vdots \\ \Delta_s^\psi \end{pmatrix}.$$

We also obtain a linear system of dimension $n_z + n_\lambda$ with matrix (3) for

$$\Delta_{s+1}^z := (\gamma^T\otimes I_{n_z}) \begin{pmatrix} \Delta Z_1 \\ \vdots \\ \Delta Z_s \\ \Delta z_1 \end{pmatrix}, \quad \Delta_{s+1}^\lambda := h(\gamma^T\widetilde{\alpha}\otimes I_{n_\lambda}) \begin{pmatrix} \Delta\widetilde{\Lambda}_0 \\ \Delta\widetilde{\Lambda}_1 \\ \vdots \\ \Delta\widetilde{\Lambda}_s \end{pmatrix}.$$

By invertibility of Q and $\widetilde{\alpha}$ we then obtain the values $\Delta Z_1, \ldots, \Delta Z_s, \Delta z_1$ and $\Delta\widetilde{\Lambda}_0, \Delta\widetilde{\Lambda}_1, \ldots, \Delta\widetilde{\Lambda}_s$ from

$$\begin{pmatrix} \Delta Z_1 \\ \vdots \\ \Delta Z_s \\ \Delta z_1 \end{pmatrix} = (Q^{-1}\otimes I_{n_z}) \begin{pmatrix} \Delta_1^z \\ \vdots \\ \Delta_s^z \\ \Delta_{s+1}^z \end{pmatrix}, \quad \begin{pmatrix} \Delta\widetilde{\Lambda}_0 \\ \Delta\widetilde{\Lambda}_1 \\ \vdots \\ \Delta\widetilde{\Lambda}_s \end{pmatrix} = \frac{1}{h}((Q\widetilde{\alpha})^{-1}\otimes I_{n_\lambda}) \begin{pmatrix} \Delta_1^\lambda \\ \vdots \\ \Delta_s^\lambda \\ \Delta_{s+1}^\lambda \end{pmatrix}.$$

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